Slave-boson mean-field theory of spin- and orbital-ordered states in the degenerate Hubbard model*

Hideo Hasegawa†
Department of Physics, Tokyo Gakugei University, Koganei, Tokyo 184, Japan.

Abstract

The mean-field theory with the use of the slave-boson functional method is generalized to take account of the spin- and orbital-ordered state in the doubly degenerate Hubbard model. Some numerical calculations are presented of the antiferromagnetic orbital-ordered state in the half-filled simple-cubic model. The orbital order in the present theory is much reduced compared with that in the Hartree-Fock approximation because of the large orbital fluctuations. From a comparison of the ground-state energy, the antiferromagnetic orbital state is shown to be unstable against the antiferromagnetic spin state, although the situation becomes reversed when the exchange interaction is *negative*.

*To be submitted to a special issue of "Foundation of Physics" celebrating the 75-th birthday of Martin Gutzwiller

†E-mail: hasegawa@u-gakugei.ac.jp

I. INTRODUCTION

In his seminal paper, Gutzwiller [1] proposed a variational approach, employing the projected wave function to take into account the effect of correlated electrons. Since the exact evaluation of the ground-state energy is difficult, he introduced an additional approximation which is now called the Gutzwiller approximation (GA). A validity of the GA was studied by Monte-Carlo method for finite-size clusters [2] [3]. It is realized that the GA becomes a better approximation for higher-dimensional systems, and it is exact in the limit of infinite dimension. The GA has been widely adopted in many area including metal-insulator transition (MIT) [4], magnetism and high-T_c superconductors (for a review of the GA of SHM see Ref. [5]).

Kotliar and Ruckenstein [21] developed the slave-boson mean-field theory by using the saddle-point approximation to the slave-boson functional-integral method. They successfully derived the antiferromagnetic solution besides the paramagnetic solution of the GA. It is shown that the GA and the slave-boson mean-field theory is equivalent.

Most of the theoretical studies based on the GA have been made for the single-band Hubbard model (SHM) for its simplicity. Actual systems, however, inevitably have the orbital degeneracy. It is necessary to investigate the role of the orbital degeneracy and the effect of Hund-rule coupling due to the exchange interaction for a better understanding on strongly correlated systems.

The first attempt to include the orbital degeneracy within the GA was made by Chao and Gutzwiller [6]. In the last few years the Hubbard model with orbital degeneracy has been extensively studied by using not only the GA-type theories [7]- [14] but also the dynamical mean-field approximation [15], [16], and Monte-Carlo simulations [17]- [19]. The original GA proposed by Chao and Gutzwiller [6] was reformulated in Refs. [7]- [10]. Lu [7] obtained the analytical expression of the critical interaction for the MIT. Okabe [8] proposed a sophisticated method in calculating te band-narrowing factor which is a difficult part in applying the GA to the degenerate band model. The first-order transition with an introduction of the exchange interaction was discussed in Ref. [9]. Bünemann, Weber and Gebhard [10] made a detailed study by using the generalized interactions.

The present author [11] proposed a slave-boson mean-field theory for the degenerate Hubbard model, by employing the slave-boson method proposed by Dorin and Schlottman [20] for the Anderson lattice model. Frésard and Kotliar [14] adopted an alternative slave-boson functional integral method. The slave-boson mean-field theory of Hasegawa [11] and Frésard and Kotliar [14] is the simple generalization of the Kotliar-Ruckenstein theory [21] for the SHM to that for the degenerate Hubbard model, and it is again equivalent to the GA [7]- [10]. The MIT in the paramagnetic state in the doubly degenerate Hubbard model (DHM) is discussed [13] [14]. Subsequently the slave-boson theory was extended and applied to the antiferromagnetic (spin) state of the half-filled DHM [12].

One of the advantages of the slave-boson mean-filed theory to the GA is that it has the wider applicability than the GA. By using the Green-function method, for example, the slave-boson mean-field theory can easily deal with the antiferromagnetic state in the SHM [21], [22] and in the doubly degenerate Hubbard model (DHM) [12]. This suggests that we can discuss a system with more complicated orderings with the slave-boson mean-field theory. It is the purpose of the present paper to generalize our theory to include the orbital ordering besides spin ordering.

The paper is organized as follows: In the next Sec. II, we present a basic formulation of our slave-boson saddle-point approximation to deal with the spin- and orbital-ordered states. Since calculations for the paramagnetic and antiferromagnetic states have been reported in our previous papers [11]- [13], we present, in Sec. III, some calculated results for the orbital-ordered state in the half-filled DHM. Section IV is devoted to conclusion and supplementary discussion.

II. FORMULATION

2.1 Basic Equations

We adopt the Hubbard model with the doubly orbital degeneracy whose Hamiltonian is given by

$$H = \sum_{\sigma}\sum_{ij}\sum_{\tau\tau'} t_{ij}^{\tau\tau'} c_{i\tau\sigma}^{\dagger} c_{j\tau'\sigma} + \frac{1}{2}\sum_{i}\sum_{(\tau,\sigma)\neq(\tau',\sigma')} U_{\tau\tau'}^{\sigma\sigma'} c_{i\tau\sigma}^{\dagger} c_{i\tau\sigma} c_{i\tau'\sigma'}^{\dagger} c_{i\tau'\sigma'} - \sum_{\sigma}\sum_{i}\sum_{\tau} (\sigma h_i + \tau g_i)\, c_{i\tau\sigma}^{\dagger} c_{i\tau'\sigma}, \tag{1}$$

where $c_{i\tau\sigma}$ is an annihilation operator of an electron with an orbital index $\tau(=\pm 1)$ and spin $\sigma\,(=\pm 1)$ on the lattice site i. The first term expresses electron hopping, which is assumed to be allowed only between the same subband: $t_{ij}^{\tau\tau'} = t_{ij}\delta_{\tau\tau'}$, for a simplicity. The on-site interaction, $U_{\tau\tau'}^{\sigma\sigma'}$, in the second term is assumed to be given by

$$U_{\tau\tau'}^{\sigma\sigma'} = U_0 = U \qquad \text{for } \tau = \tau', \sigma \neq \sigma', \tag{2}$$

$$= U_1 = U - 2J \quad \text{for } \tau \neq \tau', \sigma \neq \sigma', \tag{3}$$

$$= U_2 = U - 3J \quad \text{for } \tau \neq \tau', \sigma = \sigma', \tag{4}$$

where U and J are Coulomb and exchange interactions, respectively. In the third term of Eq.(1), h_i and g_i are the magnetic and crystal fields, respectively, at the i site.

In order to discuss the DHM with the slave-boson functional integral method, we introduce, for a given site i, sixteen slave bosons which are classified into the following five categories:

(1) e_i for the empty state;

(2) $p_{i\tau}$ for the singly occupied state with a σ-spin electron in the τ band;

(3) $d_{i0\tau}$ for the doubly occupied state with a pair of up- and down-spin electrons in the τ band; $d_{i1\tau}$ for that with an up-spin electron in the τ band and a down-spin electron in the $-\tau$ band; $d_{i2\sigma}$ for that with σ-spin electrons in the two subbands;

(4) $t_{i\tau\sigma}$ for the triply occupied state with a pair of up- and down-spin electrons in the τ band and an extra σ-spin electron in the $-\tau$ band; and

(5) f_i for the fully occupied state.

These slave bosons obey the constraint given by

$$e_i + \sum_{i\tau\sigma} p_{i\tau\sigma} + \sum_{\tau}(d_{i0\tau} + d_{i1\tau}) + \sum_{\sigma} d_{i2\sigma} + \sum_{\sigma}\sum_{\tau} t_{i\tau\sigma} + f_i = 1, \tag{5}$$

and the equivalence between fermion and boson operators is given by

$$c^{\dagger}_{i\tau\sigma}c_{i\tau\sigma} = p_{i\tau\sigma} + d_{i0\tau} + d_{i1\,\sigma\tau} + d_{i2\sigma} + t_{i\tau\sigma} + t_{i\tau-\sigma} + t_{i-\tau\sigma} + f_i. \tag{6}$$

By incorporating the conditions given by Eqs.(5) and (6) with the Lagrange multipliers, $\lambda^{(1)}_i$ and $\lambda^{(2)}_{i\tau\sigma}$, we get the partition function given as a functional integral over the coherent state of Fermi and Bose fields [11]:

$$Z = \int De \int Dp \int Dd_0 \int Dd_1 \int Dd_2 \int Dt \int Df \int D\lambda^{(1)} \int D\lambda^{(2)} \ \exp\left[-\int_0^{\beta} (L_f(t) + L_b(t)) \right], \tag{7}$$

with

$$L_f(t) = \sum_{ij}\sum_{\sigma}\sum_{\tau} z_{i\tau\sigma}\ t_{ij}\ z_{j\tau\sigma}\ c^{\dagger}_{i\tau\sigma}c_{j\tau\sigma} + \sum_{i}\sum_{\sigma}\sum_{\tau}(\frac{\partial}{\partial t} + \lambda^{(2)}_{i\tau\sigma} - \sigma\ h_i - \tau\ g_i)\ c^{\dagger}_{i\tau\sigma}c_{i\tau\sigma}. \tag{8}$$

$$\begin{aligned} L_b(t) = & \sum_i \left[\sum_{\tau}(U_0 d_{i0\tau} + U_1 d_{i1\tau}) + U_2 \sum_{\sigma}\ d_{i2\sigma} + (U_0 + U_1 + U_2) \left((\sum_{\sigma}\sum_{\tau} t_{i\tau\sigma}) + 2\ f_i \right) \right] \\ & + \sum_i (\frac{\partial}{\partial t} + \lambda^{(1)}_i) \left[e_i + \sum_{i\tau\sigma} p_{i\tau\sigma} + \sum_{\tau}(d_{i0\tau} + d_{i1\tau}) + \sum_{\sigma} d_{i2\sigma} + \sum_{\sigma}\sum_{\tau} t_{i\tau\sigma} + f_i - 1 \right] \\ & - \sum_i \sum_{\sigma}\sum_{\tau} \lambda^{(2)}_{i\tau\sigma} \left[p_{i\tau\sigma} + d_{i0\tau} + d_{i1\,\sigma\tau} + d_{i2\sigma} + t_{i\tau\sigma} + t_{i\tau-\sigma} + t_{i-\tau\sigma} + f_i \right]. \end{aligned} \tag{9}$$

Here $Dp = \Pi_i \Pi_{\sigma} \Pi_{\tau}\ d\ p_{i\tau\sigma}\ et\ al.$, β is the inverse temperature, L_f and L_b denote the terms relevant to the Fermi and Bose fields, respectively, and $z_{i\tau\sigma}$ is given by

$$\begin{aligned} z_{i\tau\sigma} = & (n_{i\tau\sigma})^{-1/2} \ (\sqrt{e_i p_{i\tau\,\sigma}} + \sqrt{p_{i\tau\,-\sigma} d_{i0\,\tau}} + \sqrt{p_{i-\tau\,-\sigma} d_{i1\,\sigma\tau}} + \sqrt{p_{i-\tau\,\sigma}\ d_{i2\,\sigma}} \\ & + \sqrt{d_{i0\,-\tau}\ t_{i-\tau\,\sigma}} + \sqrt{d_{i1\,-\sigma\tau}\ t_{i\tau\,\sigma}} + \sqrt{d_{i2\,-\sigma}\ t_{i\tau\,-\sigma}} + \sqrt{d_{i-\tau\,-\sigma}\ f_i}) \ (1 - n_{i\tau\sigma})^{-1/2}. \end{aligned} \tag{10}$$

where $n_{i\tau\sigma} = < c^{\dagger}_{i\tau\sigma}c_{i\tau\sigma} >$ and the bracket denotes the expectation value.

In discussing the spin- and/or orbital-orderded states, we make the following change of variables for $n_{i\tau\sigma}$:

$$N_i = \sum_{\sigma}\sum_{\tau} n_{i\tau\sigma}, \tag{11}$$

$$M_i = \sum_{\sigma}\sum_{\tau} \sigma\ n_{i\tau\sigma}, \tag{12}$$

$$O_i = \sum_{\sigma}\sum_{\tau} \tau\ n_{i\tau\sigma}, \tag{13}$$

$$P_i = \sum_{\sigma}\sum_{\tau} \sigma\tau\ n_{i\tau\sigma}, \tag{14}$$

where N_i, M_i, O_i and P_i denote operators relevant to the number of electrons, the magnetic moment, the orbital order and the orbital spin polarization, respectively, at a given i site. Similarly, we make the change of variables for $\lambda^{(2)}_{i\tau\sigma}$ as follows:

$$\nu_i = (1/4)\ \sum_\sigma \sum_\tau \lambda^{(2)}_{i\tau\sigma}, \tag{15}$$

$$\xi_i = (-1/4)\ \sum_\sigma \sum_\tau \sigma\ \lambda^{(2)}_{i\tau\sigma}, \tag{16}$$

$$\phi_i = (-1/4)\ \sum_\sigma \sum_\tau \tau\ \lambda^{(2)}_{i\tau\sigma}, \tag{17}$$

$$\eta_i = (-1/4)\ \sum_\sigma \sum_\tau \sigma\tau\ \lambda^{(2)}_{i\tau\sigma}, \tag{18}$$

where ν_i, ξ_i, ϕ_i and η_i stand for conjugate fields of N_i, M_i, O_i and P_i, respectively. Then $n_{i\tau\sigma}$ and $\lambda^{(2)}_{i\tau\sigma}$ are expressed by

$$n_{i\tau\sigma} = (1/4)\ (N_i + \sigma\ M_i + \tau\ O_i + \sigma\tau\ P_i) \tag{19}$$

$$\lambda^{(2)}_{i\tau\sigma} = (\nu_i - \sigma\ \xi_i - \tau\ \phi_i - \sigma\tau\ \eta_i) \tag{20}$$

Substituting Eqs.(19) and (20) to Eqs.(7)-(9) with some manipulations, we get the partition function within the static approximation, given by

$$\begin{aligned} Z = \int DN \int DM \int DO \int DP \int D\nu \int D\xi \int D\phi \int D\eta \\ \times \int Dd_0 \int Dd_1 \int Dd_2 \int Dt \int Df\ \exp(-\beta\Phi), \end{aligned} \tag{21}$$

with

$$\Phi = \Phi_0 + \Phi_1 + \Phi_2, \tag{22}$$

$$\Phi_0 = \sum_i \left[\sum_\tau (U_0 d_{i0\tau} + U_1 d_{i1\tau}) + U_2 \sum_\sigma\ d_{i2\sigma} + (U_0 + U_1 + U_2) \left((\sum_\sigma \sum_\tau t_{i\tau\sigma}) + 2\ f_i \right) \right], \tag{23}$$

$$\Phi_1 = \sum_i \left[(\varepsilon_F - \nu_i) N_i + \xi_i M_i + \phi_i O_i + \eta_i P_i \right], \tag{24}$$

$$\Phi_2 = \int d\varepsilon\ f(\varepsilon)\ (-1/\pi)\ \mathrm{Im}\ \mathrm{Tr}\ \ln G(\varepsilon). \tag{25}$$

Here $f(\varepsilon)$ is the Fermi-distribution function, ε_F the Fermi energy and $G(\varepsilon)$ is the one-particle Green function given by

$$G(\varepsilon) = (\varepsilon - H_{\mathrm{eff}})^{-1}, \tag{26}$$

where the effective slave-boson Hamiltonian, H_{eff}, is given by

$$H_{\rm eff} = \sum_{ij}\sum_{\sigma}\sum_{\tau} q^{ij}_{\tau\sigma} t_{ij} c^{\dagger}_{i\tau\sigma} c_{j\tau\sigma} + \sum_{i}\sum_{\sigma}\sum_{\tau} \left[\nu_i - \sigma(h_i + \xi_i) - \tau(g_i + \phi_i) - \sigma\tau\ \eta_i\right]\ c^{\dagger}_{i\tau\sigma} c_{i\tau\sigma}. \tag{27}$$

and the band-narrowing factor, $q^{ij}_{\tau\sigma}$, is given by

$$q^{ij}_{\tau\sigma} = z_{i\tau\sigma}\ z_{j\tau\sigma}, \tag{28}$$

with

$$z_{i\tau\sigma} = C_{i\tau\sigma}/D_{i\tau\sigma}, \tag{29}$$

$$\begin{aligned} C_{i\tau\sigma} = 16(&\sqrt{e_i p_{i\tau\ \sigma}} + \sqrt{p_{i\tau\ -\sigma} d_{i0\ \tau}} + \sqrt{p_{i-\tau\ -\sigma} d_{i1\ \sigma\tau}} + \sqrt{p_{i-\tau\ \sigma}\ d_{i2\ \sigma}} \\ &+\sqrt{d_{i0\ -\tau}\ t_{i-\tau\ \sigma}} + \sqrt{d_{i1\ -\sigma\tau}\ t_{i\tau\ \sigma}} + \sqrt{d_{i2\ -\sigma}\ t_{i\tau\ -\sigma}} + \sqrt{d_{i-\tau\ -\sigma}\ f_i}), \end{aligned} \tag{30}$$

$$D_{i\tau\sigma} = (N_i + \sigma M_i + \tau O_i + \tau\ \sigma P_i)^{1/2}\ (4 - N_i - \sigma M_i - \tau O_i - \tau\ \sigma P_i)^{1/2}. \tag{31}$$

$$e_i = 1 - N_i + \sum_{\tau}(d_{i0\tau} + d_{i1\tau}) + \sum_{\sigma} d_{i2\sigma} + 2\sum_{\sigma}\sum_{\tau} t_{i\tau\sigma} + 3f, \tag{32}$$

$$p_{i\tau\sigma} = (1/4)(N_i + \sigma\ M_i + \tau\ O_i + \sigma\tau P_i) - (d_{i0\tau} + d_{i1\ \sigma\tau} + d_{i2\sigma} + \sum_{\sigma} t_{i\tau\sigma} + t_{i-\tau\sigma} + f_i) \tag{33}$$

Since the effective transfer integral in Eq.(27) is expressed as a product form: $z_{i\tau\sigma} t_{ij} z_{j\tau\sigma}$, we can express $G(\varepsilon)$ and Φ_2 in terms of the locator defined by

$$X_{i\tau\sigma}(\varepsilon) = \left[\varepsilon - \nu_i + \sigma(h_i + \xi_i) + \tau(g + \phi_i) + \sigma\tau\eta_i\right]/r_{i\tau\sigma}, \tag{34}$$

where

$$r_{i\tau\sigma} = (z_{i\tau\sigma})^2, \tag{35}$$

explicit expressions for Φ_2 being given shortly [Eqs. (61),(62)].

By evaluating the saddle-point value of Φ, we get the slave-boson mean-field free energy given by

$$\begin{aligned} F = \sum_i &\left[\sum_{\tau}(U_0 d_{i0\tau} + U_1 d_{i1\tau}) + U_2 \sum_{\sigma}\ d_{i2\sigma} + (U_0 + U_1 + U_2)\left((\sum_{\sigma}\sum_{\tau} t_{i\tau\sigma}) + 2\ f_i\right)\right] \\ &+ \sum_i \left[(\varepsilon_F - \nu_i)N_i + \xi_i M_i + \phi_i O_i + \eta_i P_i\right] \\ &+ \int d\varepsilon\ f(\varepsilon)\ (-1/\pi)\ {\rm Im}\ {\rm Tr}\ \ln G(\varepsilon). \end{aligned} \tag{36}$$

It is noted that for a given set of parameters of U, J, T and N, the total number of electrons (per site) given by

$$N = (1/N_0)\sum_i N_i = (1/N_0)\sum_i \sum_\sigma \sum_\tau n_{i\tau\sigma}. \tag{37}$$

where N_0 is the number of lattice sites. The optinum values of N_i, M_i, O_i, P_i, ν_i, ξ_i, ϕ_i, η_i, $d_{i0\tau}$, $d_{i1\tau}$, $d_{i2\sigma}$, $t_{i\tau\sigma}$, f_i and $\varepsilon_{\rm F}$ in Eq.(36) are determined by the self-consistent equations given by Eqs.(11)-(14) and the following equations:

$$\varepsilon_F - \nu_i + \sum_\sigma \sum_\tau R_{i\tau\sigma}(\partial r_{i\tau\sigma}/\partial N_i) = 0, \tag{38}$$

$$\xi_i + \sum_\sigma \sum_\tau R_{i\tau\sigma}(\partial r_{i\tau\sigma}/\partial M_i) = 0, \tag{39}$$

$$\phi_i + \sum_\sigma \sum_\tau R_{i\tau\sigma}(\partial r_{i\tau\sigma}/\partial O_i) = 0, \tag{40}$$

$$\eta_i + \sum_\sigma \sum_\tau R_{i\tau\sigma}(\partial r_{i\tau\sigma}/\partial P_i) = 0, \tag{41}$$

$$U_0 + \sum_\sigma \sum_{\tau'} R_{i\tau'\sigma}(\partial r_{i\tau'\sigma}/\partial d_{i0\tau}) = 0, \tag{42}$$

$$U_1 + \sum_\sigma \sum_{\tau'} R_{i\tau'\sigma}(\partial r_{i\tau'\sigma}/\partial d_{i1\tau}) = 0, \tag{43}$$

$$U_2 + \sum_{\sigma'} \sum_\tau R_{i\tau\sigma'}(\partial r_{i\tau\sigma'}/\partial d_{i2\sigma}) = 0, \tag{44}$$

$$U_0 + U_1 + U_2 + \sum_{\sigma'} \sum_{\tau'} R_{i\tau'\sigma'}(\partial r_{i\tau'\sigma'}/\partial t_{i\tau\sigma}) = 0, \tag{45}$$

$$2(U_0 + U_1 + U_2) + \sum_\sigma \sum_\tau R_{i\tau\sigma}(\partial r_{i\tau\sigma}/\partial f_i) = 0, \tag{46}$$

with

$$R_{i\tau\sigma} = \partial\Phi_2/\partial r_{i\tau\sigma}. \tag{47}$$

$$n_{i\tau\sigma} = \int d\varepsilon\ f(\varepsilon)\ (-1/\pi)\ Im\ \ < i\tau\sigma \mid G(\varepsilon) \mid i\tau\sigma >, \tag{48}$$

where $r_{i\tau\sigma}$ is given by Eq.(35), and the bra $< i\tau\sigma \mid$ and ket $\mid i\tau\sigma >$ denote the σ-spin state in the τ subband at the i site.

2.2 Spin- and Orbital-Ordered States

The expression for Φ_2 given by Eq.(25) (and then $R_{i\tau\sigma}$ in Eq.(47)) depends on $G(\varepsilon)$ given by Eqs.(26) and (27) which is specified by the electronic structure and by the spin- and orbital-ordered states to be investigated. In order to discuss the spin- and/or orbital-ordered states in the paramagnetic, ferromagnetic or antiferromagnetic state on the same footing, we divide the crystal into two sublattices, A and B. We assume that for the AF wave vector Q, the relation: $\varepsilon_{k+Q} = -\varepsilon_k$ holds where ε_k is the Fourier transform of the transfer integral, t_{ij}.

The locator given by Eq.(34) at the i (j) site belonging to the A (B) lattice, is given by

$$X_{i\tau\sigma}(\varepsilon) \equiv X_{A\tau\sigma}(\varepsilon) = \left[\varepsilon - \nu_A + \sigma(h_A + \xi_A) + \tau(g_A + \phi_A) + \sigma\tau\eta_A\right]/r_{A\tau\sigma} \qquad (i \in A), \quad (49)$$

$$X_{j\tau\sigma}(\varepsilon) \equiv X_{B\tau\sigma}(\varepsilon) = \left[\varepsilon - \nu_B + \sigma(h_B + \xi_B) + \tau(g_B + \phi_B) + \sigma\tau\eta_B\right]/r_{B\tau\sigma} \qquad (j \in B). \quad (50)$$

When the spin and orbital orderings in the A and B sublattices have the simple symmetry relation such as $\nu_A = \nu_B = \nu$, $\xi_A = \pm\, \xi_B = \xi$ and $\eta_A = \pm\, \eta_B = \eta$ with $h_A = h_B = g_A = b_B = 0$, Eqs.(49) and (50) become

$$X_{A\tau\sigma}(\varepsilon) = (\varepsilon - \nu + \sigma\xi + \tau\phi + \sigma\tau\eta)/r_{A\tau\sigma} \quad (51)$$

$$X_{B\tau\sigma}(\varepsilon) = (\varepsilon - \nu + \sigma\xi + \tau\phi + \sigma\tau\eta)/r_{B\tau\sigma} \qquad \text{for F-f state,} \quad (52)$$

$$= (\varepsilon - \nu - \sigma\xi + \tau\phi - \sigma\tau\eta)/r_{B\tau\sigma} \qquad \text{for AF-f state,} \quad (53)$$

$$= (\varepsilon - \nu + \sigma\xi - \tau\phi - \sigma\tau\eta)/r_{B\tau\sigma} \qquad \text{for F-af state,} \quad (54)$$

$$= (\varepsilon - \nu - \sigma\xi - \tau\phi + \sigma\tau\eta)/r_{B\tau\sigma} \qquad \text{for AF-af state,} \quad (55)$$

with $r_{A\tau\sigma}$ and $r_{B\tau\sigma}$ given by

$$r_{i\tau\sigma} \equiv r_{A\tau\sigma} = (z_{\tau\sigma})^2, \qquad (i \in A) \quad (56)$$

$$r_{j\tau\sigma} \equiv r_{B\tau\sigma} = r_{A\tau\sigma} \qquad \text{for F-f state,} \quad (57)$$

$$= r_{A\tau-\sigma} \qquad \text{for AF-f state,} \quad (58)$$

$$= r_{A-\tau\sigma} \qquad \text{for F-af state,} \quad (59)$$

$$= r_{A-\tau-\sigma} \qquad \text{for AF-af state.} \quad (j \in B) \quad (60)$$

In Eqs.(51)-(60) "AF-f state", for example, expresses the state in which spin and orbital orders are antiferromagnetic (AF) and ferromagnetic (f), respectively [when spin (orbital) order is vanishing, it is the paramagnetic state and is referred to as P (p) state].

After a simple calculation, Φ_2 in Eq.(25) becomes

$$\Phi_2 = \int d\varepsilon\; f(\varepsilon)\; (1/\pi)\; \mathrm{Im}\; \sum_k \sum_\sigma \sum_\tau\; \ln\left(q_{\tau\sigma}^2 \left[X_{A\tau\sigma}(\varepsilon) X_{B\tau\sigma}(\varepsilon) - \varepsilon_k^2\right]\right), \quad (61)$$

with the band-narrowing factor, $q_{\tau\sigma}$, given by

$$q_{\tau\sigma} = \sqrt{r_{A\tau\sigma} r_{B\tau\sigma}}. \quad (62)$$

where $r_{A\tau\sigma}$ and $r_{B\tau\sigma}$ are given by Eqs.(56)-(60) depending on a kind of the spin and orbital orderings. The expressions for $R_{i\tau\sigma}$ and $n_{i\tau\sigma}$ given by Eqs.(47) and (48) become

$$R_{i\tau\sigma} = \int d\varepsilon\; f(\varepsilon)\; (-1/\pi)\; \mathrm{Im}\left[(\Omega_{\tau\sigma}/r_{i\tau\sigma})\; F_0(\Omega_{\tau\sigma})\right], \quad (63)$$

$$n_{i\tau\sigma} = \int d\varepsilon \; f(\varepsilon) \; \rho_{i\tau\sigma}(\varepsilon), \tag{64}$$

where $\rho_{i\tau\sigma}$ is the local density of states of electrons with spin σ in the band τ on the site i, given by

$$\begin{aligned} \rho_{i\tau\sigma}(\varepsilon) &= (-1/\pi) \text{ Im } [K_{A\tau\sigma}(\varepsilon)/r_{A\tau\sigma}] \qquad (i \in A), \\ &= (-1/\pi) \text{ Im } [K_{B\tau\sigma}(\varepsilon)/r_{B\tau\sigma}] \qquad (i \in B), \end{aligned} \tag{65}$$

with

$$K_{A\tau\sigma}(\varepsilon) = [X_{B\tau\sigma}(\varepsilon)/X_{A\tau\sigma}(\varepsilon)]^{1/2} \, F_0(\Omega_{\tau\sigma}), \tag{66}$$

$$K_{B\tau\sigma}(\varepsilon) = [X_{A\tau\sigma}(\varepsilon)/X_{B\tau\sigma}(\varepsilon)]^{1/2} \, F_0(\Omega_{\tau\sigma}), \tag{67}$$

$$\Omega_{\tau\sigma}(\varepsilon) = [X_{A\tau\sigma}(\varepsilon) \, X_{B\tau\sigma}(\varepsilon)]^{1/2}, \tag{68}$$

$$F_0(\varepsilon) = \int d\varepsilon' \rho_0(\varepsilon')/(\varepsilon - \varepsilon'), \tag{69}$$

$\rho^0(\varepsilon)$ being the unperturbed density of states. The optimum values of fields of ν, ξ, ψ and η, the order parameters of M, O and P and the occupancies, the average of the bosons of $d_{0\tau}$ *et al.*, are self-consistently determined by Eqs.(11)-(14) with Eqs.(38)-(48).

The expressions for the free energy and the self-consistent equations given by Eqs.(36) and (38)-(48) without the orbital ordering ($O = P = 0$ and $\phi = \eta = 0$) reduce to those of the GA for the P-p state [7], [8] and to that for the AF-p state [12]. Thus the present slave-boson mean-field theory becomes the generalization to the cases including both the spin- and orbital ordered states in the DHM.

2.3 Comparison with the Hartree-Fock Theory

It is worth to compare the expression for the free energy in the present theory given by Eq.(36) with that in the Hartree-Fock approximation given by

$$\begin{aligned} F_{\text{HF}} = (1/2) \sum_i [(\varepsilon_F - \nu_i) N_i + \xi_i M_i + \phi_i O_i + \eta_i P_i] \\ + \int d\varepsilon \; f(\varepsilon) \; (-1/\pi) \text{ Im } \text{ Tr } \ln G_{HF}(\varepsilon). \end{aligned} \tag{70}$$

with

$$G_{\text{HF}}(\varepsilon) = (\varepsilon - H_{\text{HF}})^{-1} \tag{71}$$

$$H_{\text{HF}} = \sum_{ij} \sum_{\sigma} \sum_{\tau} t_{ij} c^{\dagger}_{i\tau\sigma} c_{j\tau\sigma} + \sum_i \sum_{\sigma} \sum_{\tau} [\nu_i - \sigma(h_i + \xi_i) - \tau(g_i + \phi_i) - \sigma\tau \, \eta_i] \; c^{\dagger}_{i\tau\sigma} c_{i\tau\sigma}, \tag{72}$$

ν_i, ξ_i, ϕ_i and η_i being given by

$$\nu_i = (1/4)(U_0 + U_1 + U_2)N_i, \tag{73}$$

$$\xi_i = (1/4)(U_0 + U_1 - U_2)M_i, \tag{74}$$

$$\phi_i = (1/4)(-U_0 + U_1 + U_2)O_i, \tag{75}$$

$$\eta_i = (1/4)(U_0 - U_1 + U_2)P_i. \tag{76}$$

Here N_i, M_i, O_i, P_i and ε_F are determined self-consistently by Eqs.(11)-(14) with (73) -(76). It should be noted that ν_i, ξ_i, ϕ_i and η_i in the Hartree-Fock approximation are given by Eqs.(73)-(76) while those in the present theory are variationally determined by Eqs.(38)-(41). The free energy of our theory is expected to be generally lower that the Hartree-Fock free energy, as numerically shown for the P-p, AF-p and P-af cases.

III. CALCULATED RESULTS

The formalism presented in the preceding section can be applied to various types of spin- and/or orbital-ordered states. Since calculated results for P-p and AF-p states have been published in our previous papers [11]- [13], we here present some calculations only for orbitally ordered (P-af) state in order to demonstrate the feasibility of our theory.

We perform numerical calculations for the simple-cubic model with nearest-neighbor hoppings. Input parameters for our calculations are the non-interacting density of states, $\rho_0(\varepsilon)$, the Coulomb and exchange interactions, U, J, and the total number of electrons, N, which is two for the half-filled case under consideration. We employ the approximate, analytic expression for $\rho_0(\varepsilon)$ of the simple-cubic density of states [12]. The energy and the interactions are hereafter measured in units of a half of its total band width. The calculated ground-state energy without interactions ($U = J = 0$) is $\varepsilon_0 = -0.3349$, which is in good agreement with the exact value of -0.3341 [3]. Details of the calculation method is explained in Ref. [12].

A. $J = 0$ Case

We firstly discuss the case of vanishing exchange interaction ($J = 0$), for which the P-af state is equivalent to the AF-p state discussed in Ref. [12]. The U dependences of the orbital order O, band-narrowing factor q, and the energy E of the P-af state are given by those of the sublattice magnetization M, q, and E of the AF-p state shown in Figs.1, 3 and 5, respectively, of Ref. [12]. The U-dependence of the occupancies of the P-af state is obtainable from that of the AF-p state shown in Fig.4 of Ref. [12]; $d_{0a} = d_{0b} \equiv d_0$, $d_{1a} = d_{1b} \equiv d_1$, $d_{a\uparrow} = d_{b_\uparrow} \equiv d_\uparrow$, $d_{a\downarrow} = d_{b\downarrow} \equiv d_\downarrow$, $t_{a\uparrow} = t_{b\uparrow} \equiv t_\uparrow$, and $t_{a\downarrow} = t_{b\downarrow} \equiv t_\downarrow$ in Fig.4 of Ref. [12] should be read with the following changes: $d_{oa} \leftrightarrow d_{2\uparrow}$, $d_{ob} \leftrightarrow d_{2\downarrow}$, $t_{a\downarrow} \rightarrow t_{b\downarrow}$, $t_{b\downarrow} \rightarrow t_{b\uparrow}$, and $t_{b\uparrow} \rightarrow t_{a\downarrow}$, the others being the same for the AF-p and P-af states (a and b denote the two orbital bands).

B. Finite J Case

Next we introduce the exchange interaction J into our calculation. In the case of finite J, the equivalence between the AF-p and P-af states mentioned above for $J = 0$ is no more preserved. Solid curves in Fig. 1 show the J dependence of the orbital order O for U=0.5, 1.0 and 1.5. For a comparison, results of the HFA are also shown by dashed curves. With increasing the value of J, the orbital order O in the P-af state decreases. Because of the large orbital fluctuations, the orbital order in the GA is much smaller than that in the HFA, and it almost vanishes for $J > 0.05$ where the P-p state is realized. This is in contrast with the sublattice magnetization M in the AF-p state, which increase as increasing J [12]. This is easily understood because the effective fields of O and M are given by $(U - 5J)/4$ and $(U + J)/4$, respectively, in the HFA (Eqs.(2)-(4),(73),(74)).

The densities of states of the P-af state for $J = 0.02$ and 0.0 with $U = 1.0$ are shown in Figs. 2(a) and 2(b), respectively, where $\rho_{a\uparrow} = \rho_{a\downarrow} \equiv \rho_a$ and $\rho_{b\uparrow} = \rho_{b\downarrow} \equiv \rho_b$. It is noted that Fig. 2(b) for $J = 0$ expresses also the density of states of the AF-p state if we read $\rho_a \to \rho_\uparrow (= \rho_{a\uparrow} = \rho_{b\uparrow})$ and $\rho_b \to \rho_\downarrow (= \rho_{a\downarrow} = \rho_{b\downarrow})$ [12]. When the J value is increased from 0.0 to 0.02, the orbital order decreased and the polarization in the densities of states decreases as shown by Figs. 2(a) and 2(b).

Figure 3 shows the J dependence of the band-narrowing factor q for U=0.5, 1.0 and 1.5. With increasing J, q increases slightly for $U = 0.5$ while it decreases for U= 1.0 and 1.5.

The J dependence of the occupancies is shown in Fig.4, where from the symmetry, we get $d_{2\uparrow} = d_{2\downarrow} \equiv d_2$, $t_{a\uparrow} = t_{a\downarrow} \equiv t_a$ and $t_{b\uparrow} = t_{b\downarrow} \equiv t_b$. When J is increased, d_{ob}, d_{1a}, d_{1b}, t_a and f increase whereas d_{0a} and d_{0b} decrease. At $J > 0.05$, the system becomes the P-p state where $d_{0a} = d_{0b}$ and $t_a = t_b$ (see Fig. 1).

In order to investigate the relative stability between the AF-p and P-af states, we calculate their total energies E, which are shown in Fig. 5. The bold (thin) solid curve expresses E of the AF-p state in the GA (HFA), and the bold (thin) dashed curve E of the P-af state in the GA (HFA). For $J = 0$, the AF-p and P-af states have the same total energy. We note that for all the J values investigated, E in the GA is always lower than that in the HFA for the Af-P and p-AF states, as well as for the P-p state [11], [12]. For finite (positive) J, the energy of the AF-p state is lower than that of the P-af state both in the GA and HFA.

IV. CONCLUSION AND DISCUSSION

To summarize, we have developed the theory of the spin- and orbital-ordered states in the DHM, generalizing our slave-boson mean-field theory [11]. In order to demonstrate the feasibility of our theory, we have presented numerical calculations of the antiferromagnetic orbital (P-af) state, showing the J dependences of the orbital order O, the band narrowing factor q and the occupancies. From the calculation of the total energy E, the antiferromagnetic orbital (P-af) state is shown to be unstable against the antiferromagnetic spin (AF-p) state except for $J = 0$ for which the both states are energetically degenerate.

In order to more investigate the role of the exchange interaction on orbital order in the DHM, we have made numerical calculations also for the *negative* J, although J is conventionally taken to be positive. We notice in Fig.1 that for the negative exchange interaction,

the orbital order O is considerably increased: we cannot obtain the solution at $J < 0.048$ ($J < 0.014$) for $U = 1.0$ ($U = 1.5$). This increase in O is induced by a significant increase in d_{0a}, as shown in Fig. 4. As was discussed in Ref. [12], the negative exchange interaction is not favorable for the sublattice magnetization M in the AF-p state. Then the increase in O and the decrease in M for the negative J lead to the P-af state to be more stable than the AF-p state, as the energy calculation shows in Fig. 5.

We previously showed from a comparison between the calculations using the GA [23] and the variational Monte-Calro method [3] that the GA is a fairly good approximation for the one-, two- and three-dimensional simple SHM (the GA is exact for infinite dimensional SHM). We expect that this would hold also for the DHM although no variational calculations for the DHM have been reported yet. We can apply our theory to states in which both spin and orbital orderings coexit such as the AF-f and F-f states. A study of the N-U phase diagram (N: electron number, U: interaction) of the simple-cubic DHM, as was made within the HFA [24], will be interesting. It would be also promising to investigate the temperature-interaction phase diagram of the DHM, by generalizing our approach [22] [25] in which the effects of electron correlation and thermal spin fluctuations are properly taken into account.

ACKNOWLEDGEMENTS

It is my great pleasure to dedicate the present paper to Dr. Martin Gutzwiller on the occasion of his 75th birthday. This work has been supported partially by a Grant-in-Aid for Scientific Researach (B) from the Ministry of Education, Science, Sports and Culture of Japan.

REFERENCES

[1] M. C. Gutzwiller, Phys. Rev. Lett. **10**, 159 (1963); Phys. Rev. **137**, A1726 (1965).
[2] T. A. Kaplan, P. Horsch and P. Fulde, Phys. Rev. Lett. **49**, 889 (1982).
[3] H. Yokoyama and H. Shiba, J. Phys. Soc. Jpn. **56**, 1490 (1987); *ibd* **56**, 3582 (1987).
[4] W. F. Brinkman and T. M. Rice, Phys. Rev. B **2**, 4302 (1970).
[5] F. Gebhard, 'The Mott Metal-Insulator Transition- Models and Mehtods', Springer Tracts in Modern Physcs, Vol. 137 (Springer, Berlin 1997).
[6] K. A. Chao and M. C. Gutzwiller, Phys. Rev. B **4**, 4034 (1971).
[7] J. P. Lu, Phys. Rev. B **49**, 5687 (1994).
[8] T. Okabe, J. Phys. Soc. Jpn. **65**, 1056 (1996).
[9] J. Bünemann and W. Weber, Phys. Rev. B **55**, R4011 (1997).
[10] J. Bünemann, W. Weber, and F. Gebhard, Phys. Rev. B **57**, 6896 (1998).
[11] H. Hasegawa, J. Phys. Soc. Jpn. **66**, 1391 (1997).
[12] H. Hasegawa, Phys. Rev. B **56**, 1196 (1997).
[13] H. Hasegawa, J. Phys. Soc. Jpn. **66**, 3522 (1997).
[14] R. Frésard and G. Kotliar, Phys. Rev. B **56**, 12909 (1997).
[15] G. Kotliar and H. Kajueter, Phys. Rev. B **54**, R14221 (1996).
[16] M. J. Rozenberg, Phys. Rev. B **55** R4855 (1997).
[17] W. Gill and D. J. Scalapino, Phys. Rev. B **35**, 215 (1987).
[18] J. E. Han, M. Jarrel, and D. L. Cox, Phys. Rev. B **58**, 14a99 (1998).
[19] Y. Motome and M. Imada, J. Phys. Jpn. **67**, 3199 (1998).
[20] V. Dorin and P. Schlottmann, Phys. Rev. **47**, 5095 (1993).
[21] G. Kotliar and A. E. Ruckenstein, Phys. Rev. Lett. **57**, 1362 (1986).
[22] H. Hasegawa, J. Phys. Cond. Matter. **1**, 9325 (1989);
[23] H. Hasegawa, Phys. Rev. B **41**, 9168 (1990).
[24] S. Inagaki and R. Kubo, Int. J. Mag. **4**, 139 (1973).
[25] H. Hasegawa, Prog. Theor. Phys. Suppl.**101**, 463 (1990).

FIGURES

FIG. 1. The J dependence of the orbital order O in the P-af state calculated by the GA (solid curves) and HFA (dashed curves)

FIG. 2. The local densities of state in the P-af state for (a) $J = 0.02$ and (b) $J = 0.0$ with $U = 1.0$: $\rho_{a\uparrow} = \rho_{a\downarrow} \equiv \rho_a$ (solid curves) and $\rho_{b\uparrow} = \rho_{b\downarrow} \equiv \rho_a$ (dashed curves).

FIG. 3. The J dependence of the band-narrowing factor q in the P-af state.

FIG. 4. The J dependence of the occupancies in the P-af state: $d_{2\uparrow} = d_{2\downarrow} \equiv d_2$, $t_{a\uparrow} = t_{a\downarrow} \equiv t_a$ and $t_{b\uparrow} = t_{b\downarrow} \equiv t_b$.

FIG. 5. The J dependence of the total energies E of the AF-p state in the GA (bold, solid curve) and HFA (thin, solid curve), and E of the P-af state in the GA (bold, dashed curve) and HFA (thin, dashed curve).

This figure "fig1.gif" is available in "gif" format from:

http://arXiv.org/ps/cond-mat/0005271v1